

Stability of ADI schemes for multidimensional diffusion equations with mixed derivative terms

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Abstract

In this paper the unconditional stability of four well-known ADI schemes is analyzed in the application to time-dependent multidimensional diffusion equations with mixed derivative terms. Necessary and sufficient conditions on the parameter θ of each scheme are obtained that take into account the actual size of the mixed derivative coefficients. Our results generalize results obtained previously by Craig & Sneyd (1988) and In 't Hout & Welfert (2009). Numerical experiments are presented illustrating our main theorems.

1 Introduction

1.1 Multidimensional diffusion equations with mixed derivative terms

This paper is concerned with stability in the numerical solution of initial-boundary value problems for time-dependent multidimensional diffusion equations containing mixed spatial-derivative terms,

$$\frac{\partial u}{\partial t} = \sum_{i \neq j} d_{ij} u_{x_i x_j} + d_{11} u_{x_1 x_1} + d_{22} u_{x_2 x_2} + \cdots + d_{kk} u_{x_k x_k} \quad (1.1)$$

Here $k \geq 2$ is any given integer and $D = (d_{ij})_{1 \leq i, j \leq k}$ denotes any given real, symmetric, positive semidefinite $k \times k$ matrix. The spatial domain is taken as $\Omega = (0, 1)^k$ and $t > 0$.

Multidimensional diffusion equations with mixed derivative terms play an important role, notably, in the field of financial option pricing theory. Here these terms represent correlations between underlying stochastic processes, such as for asset prices, volatilities or interest rates, see e.g. [1, 16, 17, 18].

In this paper we consider for given $\gamma \in [0, 1]$ the following useful condition on the relative size of the mixed derivative coefficients,

$$|d_{ij}| \leq \gamma \sqrt{d_{ii} d_{jj}} \quad \text{whenever } 1 \leq i, j \leq k, i \neq j. \quad (1.2)$$

Clearly, $\gamma = 0$ yields the smallest possible mixed derivative coefficients; they all vanish in this case. Subsequently, $\gamma = 1$ admits the largest possible mixed derivative coefficients, given that matrix D is positive semidefinite. In most applications in financial mathematics it turns out that (1.2) holds with certain known $0 < \gamma < 1$. More precisely, such γ can be determined from the pertinent correlation coefficients. The aim of our present paper is to effectively use this knowledge about γ in the stability analysis of numerical schemes, discussed below, so as to arrive at weaker sufficient stability conditions than those obtained when considering $\gamma = 1$.

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1.2 Alternating Direction Implicit schemes

Semidiscretization of initial-boundary value problems for multidimensional diffusion equations (1.1) leads to initial value problems for very large systems of stiff ordinary differential equations,

$$U'(t) = AU(t) + g(t) \quad (t \geq 0), \quad U(0) = U_0. \quad (1.3)$$

Here A is a given real $m \times m$ matrix and $g(t)$ (for $t \geq 0$) and U_0 are given real $m \times 1$ vectors. For the efficient numerical solution of (1.3), splitting schemes of the Alternating Direction Implicit (ADI) type form an attractive means. These schemes employ a splitting of the matrix A that corresponds to the different spatial directions, leading to a substantial reduction in the amount of computational work per time step compared to common implicit methods such as Crank–Nicolson. ADI schemes constitute a popular class of numerical methods for multidimensional equations in financial mathematics, where mixed derivative terms are ubiquitous.

Originally ADI schemes were proposed and analyzed for equations without mixed derivatives, see e.g. [2, 4, 5]. To formulate ADI schemes in the presence of mixed derivative terms, consider a splitting of the matrix A into

$$A = A_0 + A_1 + \cdots + A_k, \quad (1.4)$$

where A_0 represents all mixed derivative terms in (1.1) and A_j represents the derivative term in the j -th spatial direction for $j = 1, 2, \dots, k$. Split the vector function g in an analogous way,

$$g = g_0 + g_1 + \cdots + g_k,$$

and define

$$F(t, \xi) = A\xi + g(t) \quad \text{and} \quad F_j(t, \xi) = A_j\xi + g_j(t) \quad \text{whenever } t \geq 0, \xi \in \mathbb{R}^m, 0 \leq j \leq k.$$

Let parameter $\theta > 0$ be given. Let time step $\Delta t > 0$ and temporal grid points $t_n = n\Delta t$ with integer $n \geq 0$. For the numerical solution of the semidiscrete system (1.3), we study in this paper four ADI schemes, each successively generating for $n = 1, 2, 3, \dots$ approximations U_n to $U(t_n)$:

Douglas (Do) scheme

$$\begin{cases} Y_0 = U_{n-1} + \Delta t F(t_{n-1}, U_{n-1}), \\ Y_j = Y_{j-1} + \theta \Delta t (F_j(t_n, Y_j) - F_j(t_{n-1}, U_{n-1})), \quad j = 1, 2, \dots, k, \\ U_n = Y_k \end{cases} \quad (1.5)$$

Craig–Sneyd (CS) scheme

$$\begin{cases} Y_0 = U_{n-1} + \Delta t F(t_{n-1}, U_{n-1}), \\ Y_j = Y_{j-1} + \theta \Delta t (F_j(t_n, Y_j) - F_j(t_{n-1}, U_{n-1})), \quad j = 1, 2, \dots, k, \\ \tilde{Y}_0 = Y_0 + \frac{1}{2} \Delta t (F_0(t_n, Y_k) - F_0(t_{n-1}, U_{n-1})), \\ \tilde{Y}_j = \tilde{Y}_{j-1} + \theta \Delta t (F_j(t_n, \tilde{Y}_j) - F_j(t_{n-1}, U_{n-1})), \quad j = 1, 2, \dots, k, \\ U_n = \tilde{Y}_k \end{cases} \quad (1.6)$$

Modified Craig-Sneyd (MCS) scheme

$$\left\{ \begin{array}{l} Y_0 = U_{n-1} + \Delta t F(t_{n-1}, U_{n-1}), \\ Y_j = Y_{j-1} + \theta \Delta t (F_j(t_n, Y_j) - F_j(t_{n-1}, U_{n-1})), \quad j = 1, 2, \dots, k, \\ \hat{Y}_0 = Y_0 + \theta \Delta t (F_0(t_n, Y_k) - F_0(t_{n-1}, U_{n-1})), \\ \tilde{Y}_0 = \hat{Y}_0 + (\frac{1}{2} - \theta) \Delta t (F(t_n, Y_k) - F(t_{n-1}, U_{n-1})), \\ \tilde{Y}_j = \tilde{Y}_{j-1} + \theta \Delta t (F_j(t_n, \tilde{Y}_j) - F_j(t_{n-1}, U_{n-1})), \quad j = 1, 2, \dots, k, \\ U_n = \tilde{Y}_k \end{array} \right. \quad (1.7)$$

Hundsdorfer-Verwer (HV) scheme

$$\left\{ \begin{array}{l} Y_0 = U_{n-1} + \Delta t F(t_{n-1}, U_{n-1}), \\ Y_j = Y_{j-1} + \theta \Delta t (F_j(t_n, Y_j) - F_j(t_{n-1}, U_{n-1})), \quad j = 1, 2, \dots, k, \\ \tilde{Y}_0 = Y_0 + \frac{1}{2} \Delta t (F(t_n, Y_k) - F(t_{n-1}, U_{n-1})), \\ \tilde{Y}_j = \tilde{Y}_{j-1} + \theta \Delta t (F_j(t_n, \tilde{Y}_j) - F_j(t_n, Y_k)), \quad j = 1, 2, \dots, k, \\ U_n = \tilde{Y}_k. \end{array} \right. \quad (1.8)$$

A study of the above four ADI schemes shows that the A_0 part, representing all mixed derivative terms, is always treated in an *explicit* fashion. In line with the original ADI idea, the A_j parts for $j = 1, 2, \dots, k$ are successively treated in an *implicit* fashion.

In its general form (1.5) the Douglas scheme has been considered e.g. in [12, 14]. Special instances include the well-known ADI schemes of Douglas & Rachford [5], where $F_0 = 0$ and $\theta = 1$, and of Brian [2] and Douglas [4], where $F_0 = 0$ and $\theta = \frac{1}{2}$. McKee & Mitchell [15] first proposed the Do scheme for equations (1.1) where a mixed derivative term is present, with $k = 2$.

It is readily shown that if A_0 is nonzero then the classical order of consistency¹ of the Do scheme is just one, for any given θ .

The CS, MCS and HV schemes can be viewed as different extensions to the Do scheme. They each perform a second explicit prediction stage followed by k implicit correction stages. The CS scheme was introduced in [3] and attains a classical order equal to two (independently of A_0) if $\theta = \frac{1}{2}$. The MCS scheme was defined in [11] and possesses a classical order equal to two for any given θ . Note that the CS and MCS schemes are identical if $\theta = \frac{1}{2}$. The HV scheme was constructed in [13] and was proposed for equations with mixed derivative terms in [10]. Like the MCS scheme, the HV scheme possesses the favorable property of having a classical order equal to two for any given θ .

For the stability analysis in this paper the following linear scalar *test equation* is relevant,

$$U'(t) = (\lambda_0 + \lambda_1 + \dots + \lambda_k)U(t), \quad (1.9)$$

with complex constants λ_j ($0 \leq j \leq k$). Application of any given ADI scheme in the case of test equation (1.9) gives rise to a linear iteration of the form

$$U_n = M(z_0, z_1, \dots, z_k) U_{n-1}.$$

¹That is, the order for fixed, nonstiff ODEs.

Here M is a given, fixed, multivariate rational function and $z_j = \Delta t \lambda_j$ ($0 \leq j \leq k$). The iteration is stable if

$$|M(z_0, z_1, \dots, z_k)| \leq 1. \quad (1.10)$$

Write

$$z = z_1 + z_2 + \dots + z_k \quad \text{and} \quad p = (1 - \theta z_1)(1 - \theta z_2) \dots (1 - \theta z_k). \quad (1.11)$$

For the schemes (1.5), (1.6), (1.7), (1.8) it is readily verified that $M = R, \tilde{S}, S, T$, respectively, where

$$R(z_0, z_1, \dots, z_k) = 1 + \frac{z_0 + z}{p}, \quad (1.12)$$

$$\tilde{S}(z_0, z_1, \dots, z_k) = 1 + \frac{z_0 + z}{p} + \frac{1}{2} \frac{z_0(z_0 + z)}{p^2}, \quad (1.13)$$

$$S(z_0, z_1, \dots, z_k) = 1 + \frac{z_0 + z}{p} + \theta \frac{z_0(z_0 + z)}{p^2} + \left(\frac{1}{2} - \theta\right) \frac{(z_0 + z)^2}{p^2}, \quad (1.14)$$

$$T(z_0, z_1, \dots, z_k) = 1 + 2 \frac{z_0 + z}{p} - \frac{z_0 + z}{p^2} + \frac{1}{2} \frac{(z_0 + z)^2}{p^2}. \quad (1.15)$$

1.3 Finite difference discretization

For the semidiscretization of (1.1) we replace all spatial derivatives by second-order central finite differences on a rectangular grid with constant mesh width $\Delta x_i > 0$ in the x_i -direction ($1 \leq i \leq k$):

$$(u_{x_i x_i})_\ell \approx \frac{u_{\ell+e_i} - 2u_\ell + u_{\ell-e_i}}{(\Delta x_i)^2}, \quad (1.16a)$$

$$(u_{x_i x_j})_\ell \approx \frac{(1 + \beta_{ij})(u_{\ell+e_i+e_j} + u_{\ell-e_i-e_j}) - (1 - \beta_{ij})(u_{\ell-e_i+e_j} + u_{\ell+e_i-e_j})}{4\Delta x_i \Delta x_j} + \frac{\beta_{ij}(4u_\ell - 2(u_{\ell+e_i} + u_{\ell+e_j} + u_{\ell-e_i} + u_{\ell-e_j}))}{4\Delta x_i \Delta x_j}, \quad i \neq j. \quad (1.16b)$$

Here $\ell = (\ell_1, \ell_2, \dots, \ell_k)$ and the unit vectors e_1, e_2, \dots, e_k denote multi-indices, u_ℓ stands for $u(\ell_1 \Delta x_1, \ell_2 \Delta x_2, \dots, \ell_k \Delta x_k, t)$ and β_{ij} ($1 \leq i \neq j \leq k$) are given real parameters with $\beta_{ij} = \beta_{ji}$. The righthand side of (1.16b) is the most general second-order finite difference formula for the mixed derivative $u_{x_i x_j}$ that is based on a centered 9-point stencil. If $\beta_{ij} = 0$, then (1.16b) reduces to the standard 4-point formula

$$(u_{x_i x_j})_\ell \approx \frac{u_{\ell+e_i+e_j} + u_{\ell-e_i-e_j} - u_{\ell-e_i+e_j} - u_{\ell+e_i-e_j}}{4\Delta x_i \Delta x_j}.$$

In the literature also the choices $\beta_{ij} = -1$ and $\beta_{ij} = 1$ are frequently considered.

1.4 Stability analysis and outline of this paper

The aim of this paper is to investigate the stability of the four ADI schemes (1.5)–(1.8) in the application to semidiscretized multidimensional diffusion equations (1.1) where the condition (1.2) on the size of the mixed derivative coefficients is effectively taken into account. Our stability analysis is equivalent to the well-known von Neumann (Fourier) analysis. Accordingly, (1.1) is considered with constant diffusion matrix D and periodic boundary condition and stability pertains to the l_2 -norm. The obtained semidiscrete matrices A_j ($0 \leq j \leq k$) are then all normal and commuting and can therefore be unitarily diagonalized by a single matrix. For any given ADI scheme, one thus arrives at the stability requirement (1.10) with λ_j eigenvalues of the matrices A_j ($0 \leq j \leq k$).

Upon substituting discrete Fourier modes into (1.16), it is readily shown that the scaled eigenvalues z_j are given by

$$z_0 = \sum_{i \neq j} r_{ij} d_{ij} [-\sin \phi_i \sin \phi_j + \beta_{ij}(1 - \cos \phi_i)(1 - \cos \phi_j)], \quad (1.17a)$$

$$z_j = -2r_{jj}d_{jj}(1 - \cos \phi_j), \quad j = 1, 2, \dots, k. \quad (1.17b)$$

The angles ϕ_j are integer multiples of $2\pi/m_j$ with m_j the dimension of the grid in the x_j -direction ($1 \leq j \leq k$). Further,

$$r_{ij} = \frac{\Delta t}{\Delta x_i \Delta x_j} \quad \text{for } 1 \leq i, j \leq k.$$

Stability results for ADI schemes pertinent to (1.2) in the case of $\gamma = 1$ were derived by Craig & Sneyd [3] for the Do and CS schemes and by In 't Hout & Welfert [11] for the MCS and HV schemes. For any given scheme, both necessary and sufficient conditions on its parameter θ were obtained such that the stability requirement (1.10) with (z_0, z_1, \dots, z_k) given by (1.17) is unconditionally fulfilled, i.e., for all $\Delta t > 0$ and all $\Delta x_i > 0$ ($1 \leq i \leq k$).

The stability analysis of ADI schemes based on (1.2) with *arbitrary* given $\gamma \in [0, 1]$ was recently started in In 't Hout & Mishra [8]. For the MCS scheme and $k = 2$, the useful result was proved here that the lower bound $\theta \geq \max\{\frac{1}{4}, \frac{1}{6}(\gamma + 1)\}$ is sufficient for unconditional stability (whenever $0 \leq \gamma \leq 1$).

The present paper substantially extends the work of [3, 8, 11] reviewed above. Section 2 contains the two main results of this paper. The first main result is Theorem 2.3, which provides for each of the Do, CS, MCS, HV schemes in $k = 2$ and $k = 3$ spatial dimensions a *sufficient* condition on the parameter θ for unconditional stability under (1.2) for arbitrary given $\gamma \in [0, 1]$. The second main result is Theorem 2.4. This yields for any of the four ADI schemes, any spatial dimension $k \geq 2$ and any $\gamma \in [0, 1]$ a *necessary* condition on θ for unconditional stability under (1.2). For each scheme, the obtained necessary and sufficient conditions coincide if $k = 2$ or $k = 3$. Section 3 presents numerical illustrations to the two main theorems. The final Section 4 gives conclusions and issues for future research.

2 Main results

In the following we always make the minor assumption that the matrix $B = (-\beta_{ij})_{1 \leq i, j \leq k}$ with $\beta_{ii} = -1$ ($1 \leq i \leq k$) is positive semidefinite. Thus, in particular, $|\beta_{ij}| \leq 1$ for all i, j . We note that this assumption on B is weaker than the corresponding assumption that was made in [11].

2.1 Preliminaries

This section gives two lemmas that shall be used in the proofs of the main results below.

Lemma 2.1 *Let α, δ be given real numbers with $0 < \delta \leq 4$. Consider the polynomial*

$$P(u, v, w) = \alpha + u^2 + v^2 + w^2 + uvw - \delta(u + v + w) \quad \text{for } u, v, w \in \mathbb{R}.$$

Then

$$P(u, v, w) \geq 0 \quad \text{whenever } u \geq 0, v \geq 0, w \geq 0$$

if and only if

$$(\delta + 1)(3 - 2\sqrt{\delta + 1}) \geq 1 - \alpha \quad \text{and} \quad \delta^2 \leq 2\alpha. \quad (2.1)$$

Proof The critical points (u, v, w) of P are given by the equations

$$2u + vw = 2v + uw = 2w + uv = \delta.$$

A straightforward analysis, using $0 < \delta \leq 4$, shows that there is precisely one critical point in the domain $u > 0, v > 0, w > 0$, and it is given by $u = v = w = \sqrt{\delta + 1} - 1 =: u^*$. Inserting this into P and rewriting yields

$$\begin{aligned} P(u^*, u^*, u^*) &= (u^* + 1)^3 - 3(\delta + 1)u^* + \alpha - 1 \\ &= (\sqrt{\delta + 1})^3 - 3(\delta + 1)(\sqrt{\delta + 1} - 1) + \alpha - 1 \\ &= (\delta + 1)(3 - 2\sqrt{\delta + 1}) + \alpha - 1. \end{aligned}$$

Hence $P(u^*, u^*, u^*) \geq 0$ if and only if the first inequality in (2.1) holds.

Consider next the polynomial P on the boundary of the pertinent domain. It is clear that $P(u, v, w) \geq 0$ if $u, v, w \rightarrow \infty$. Next, on the boundary part $u \geq 0, v \geq 0, w = 0$ there holds

$$\begin{aligned} P(u, v, 0) &= \alpha + u^2 + v^2 - \delta(u + v) \\ &= (u - \tfrac{1}{2}\delta)^2 + (v - \tfrac{1}{2}\delta)^2 + \alpha - \tfrac{1}{2}\delta^2. \end{aligned}$$

Thus $P(u, v, 0) \geq 0$ (whenever $u \geq 0, v \geq 0$) if and only if the second inequality in (2.1) holds. By symmetry, the result for the other two boundary parts is the same, which completes the proof. ■

The subsequent analysis relies upon four key properties of the scaled eigenvalues (1.17).

Lemma 2.2 *Let z_0, z_1, \dots, z_k be given by (1.17). Let $\gamma \in [0, 1]$ and assume (1.2) holds. Then:*

$$\text{all } z_j \text{ are real,} \tag{2.2a}$$

$$z_j \leq 0 \text{ for } 1 \leq j \leq k, \tag{2.2b}$$

$$z + z_0 \leq 0, \tag{2.2c}$$

$$|z_0| \leq \gamma \sum_{i \neq j} \sqrt{z_i z_j}. \tag{2.2d}$$

Proof Properties (2.2a), (2.2b) are obvious. We consider (2.2c) and (2.2d). Using $r_{ij} = \sqrt{r_{ii}r_{jj}}$ and the simple identity

$$(\sin \phi)^2 + (1 - \cos \phi)^2 = 2(1 - \cos \phi)$$

one readily verifies that

$$-(z + z_0) = \sum_{i,j=1}^k r_{ij} d_{ij} [\sin \phi_i \sin \phi_j - \beta_{ij}(1 - \cos \phi_i)(1 - \cos \phi_j)] = \mathbf{u}^T D \mathbf{u} + \mathbf{v}^T (D \circ B) \mathbf{v},$$

where \circ denotes the Hadamard product of two matrices and

$$\mathbf{u} = (\sqrt{r_{jj}} \sin \phi_j)_{1 \leq j \leq k}, \quad \mathbf{v} = (\sqrt{r_{jj}} (1 - \cos \phi_j))_{1 \leq j \leq k}.$$

It is well-known that the Hadamard product of two positive semidefinite matrices is also positive semidefinite, see e.g. [7], and hence, $z + z_0 \leq 0$ is obtained.

Next, using the Cauchy-Schwarz inequality and $|\beta_{ij}| \leq 1$, it directly follows that

$$|\sin \phi_i \sin \phi_j - \beta_{ij}(1 - \cos \phi_i)(1 - \cos \phi_j)| \leq \sqrt{2(1 - \cos \phi_i)} \cdot \sqrt{2(1 - \cos \phi_j)}.$$

Together with (1.2) this yields

$$|z_0| \leq \gamma \sum_{i \neq j} \sqrt{r_{ii}r_{jj}} \sqrt{d_{ii}d_{jj}} \sqrt{2(1 - \cos \phi_i)} \cdot \sqrt{2(1 - \cos \phi_j)} = \gamma \sum_{i \neq j} \sqrt{z_i z_j}.$$

■

In the following we shall use the notation $y_j = \sqrt{-\theta z_j}$ (for $1 \leq j \leq k$). Then

$$p = \prod_{j=1}^k (1 + y_j^2) \geq 1 \quad \text{and} \quad z = -\frac{1}{\theta} \sum_{j=1}^k y_j^2 \quad (2.3)$$

and by (2.2d) there holds

$$z + z_0 \geq z - |z_0| \geq \sum_{j=1}^k z_j - \gamma \sum_{i \neq j} \sqrt{z_i z_j} = -\frac{1}{\theta} \left(\sum_{j=1}^k y_j^2 + \gamma \sum_{i \neq j} y_i y_j \right). \quad (2.4)$$

2.2 Two main theorems

The first main result gives sufficient conditions on θ for unconditional stability of each of the Do, CS, MCS, HV schemes in the application to (1.1) for $k = 2$ or $k = 3$ under condition (1.2) with arbitrary given γ .

Theorem 2.3 *Consider equation (1.1) for $k = 2$ or $k = 3$ with symmetric positive semidefinite matrix D and periodic boundary condition. Let $\gamma \in [0, 1]$ and assume (1.2) holds. Let (1.3), (1.4) be obtained by central second-order FD discretization and splitting as described in Section 1. Then for the following parameter values θ the Do, CS, MCS, HV schemes are unconditionally stable when applied to (1.3), (1.4):*

- *Do scheme:*

$$\theta \geq \frac{1}{2} \quad (\text{if } k = 2) \quad \text{and} \quad \theta \geq \max \left\{ \frac{1}{2}, \frac{2(2\gamma + 1)}{9} \right\} \quad (\text{if } k = 3);$$

- *CS scheme:*

$$\theta \geq \frac{1}{2} \quad (\text{if } k = 2 \text{ or } k = 3);$$

- *MCS scheme:*

$$\theta \geq \max \left\{ \frac{1}{4}, \frac{\gamma + 1}{6} \right\} \quad (\text{if } k = 2) \quad \text{and} \quad \theta \geq \max \left\{ \frac{1}{4}, \frac{2(2\gamma + 1)}{13} \right\} \quad (\text{if } k = 3);$$

- *HV scheme:*

$$\theta \geq \max \left\{ \frac{1}{4}, \frac{\gamma + 1}{4 + 2\sqrt{2}} \right\} \quad (\text{if } k = 2) \quad \text{and} \quad \theta \geq \max \left\{ \frac{1}{4}, \frac{2\gamma + 1}{4 + 2\sqrt{3}} \right\} \quad (\text{if } k = 3).$$

Proof The proofs for the four schemes are similar. In view of this, we shall consider here the HV scheme and leave the proofs for the Do, CS and MCS schemes to the reader.²

Using the properties (2.2a)–(2.2c) of the scaled eigenvalues, it is readily seen that for $M = T$ the stability requirement (1.10) is equivalent to

$$2p^2 + (2p - 1)(z_0 + z) + \frac{1}{2}(z_0 + z)^2 \geq 0, \quad (2.5a)$$

$$2p - 1 + \frac{1}{2}(z_0 + z) \geq 0. \quad (2.5b)$$

Condition (2.5a) is always fulfilled since the discriminant $(2p - 1)^2 - 4p^2 = -4p + 1 < 0$. Subsequently, using (2.3) and (2.4) it is easily seen that if there exists $\kappa > 0$ such that

$$2 \prod_{j=1}^k (1 + y_j^2) - 1 - \kappa \left(\sum_{j=1}^k y_j^2 + \gamma \sum_{i \neq j} y_i y_j \right) \geq 0 \quad (2.6)$$

²See, however, [8] for the MCS scheme if $k = 2$.

for all $y_j \geq 0$ ($1 \leq j \leq k$), then condition (2.5b) is fulfilled whenever $\theta \geq 1/(2\kappa)$.

For $k = 2$ the inequality (2.6) reads

$$1 + 2(y_1^2 + y_2^2 + y_1^2 y_2^2) - \kappa(y_1^2 + y_2^2 + 2\gamma y_1 y_2) \geq 0,$$

and this can be rewritten as

$$(2 - \kappa)(y_1 - y_2)^2 + 2(y_1 y_2 + 1 - \frac{1}{2}\kappa - \frac{1}{2}\kappa\gamma)^2 + 1 - 2(1 - \frac{1}{2}\kappa - \frac{1}{2}\kappa\gamma)^2 \geq 0.$$

Hence, the inequality is satisfied if

$$\kappa \leq 2 \quad \text{and} \quad \sqrt{2}|1 - \frac{1}{2}\kappa - \frac{1}{2}\kappa\gamma| \leq 1,$$

which is equivalent to

$$\frac{2 - \sqrt{2}}{\gamma + 1} \leq \kappa \leq \min \left\{ 2, \frac{2 + \sqrt{2}}{\gamma + 1} \right\}.$$

Selecting the rightmost value for κ , yields that (2.5b) holds for $k = 2$ whenever

$$\theta \geq \max \left\{ \frac{1}{4}, \frac{\gamma + 1}{4 + 2\sqrt{2}} \right\}.$$

For $k = 3$ the inequality (2.6) reads

$$1 + (2 - \kappa) \sum_{j=1}^3 y_j^2 + 2 \sum_{i < j} y_i^2 y_j^2 + 2y_1^2 y_2^2 y_3^2 - 2\kappa\gamma \sum_{i < j} y_i y_j \geq 0,$$

which, by the identity

$$\sum_{i < j} (y_i - y_j)^2 = 2 \sum_{j=1}^3 y_j^2 - 2 \sum_{i < j} y_i y_j,$$

is equivalent to

$$1 + \frac{1}{2}(2 - \kappa) \sum_{i < j} (y_i - y_j)^2 + 2 \sum_{i < j} y_i^2 y_j^2 + 2y_1^2 y_2^2 y_3^2 + (2 - \kappa - 2\kappa\gamma) \sum_{i < j} y_i y_j \geq 0.$$

Let $u = y_1 y_2$, $v = y_1 y_3$, $w = y_2 y_3$. Then $u, v, w \geq 0$ and the above inequality can be written as

$$\frac{1}{2}(2 - \kappa) \sum_{i < j} (y_i - y_j)^2 + 2P(u, v, w) \geq 0,$$

where

$$P(u, v, w) = \alpha + u^2 + v^2 + w^2 + uvw - \delta(u + v + w)$$

with

$$\alpha = \frac{1}{2} \quad \text{and} \quad \delta = \frac{1}{2}\kappa + \kappa\gamma - 1.$$

Hence, if $\kappa \leq 2$ and $P(u, v, w) \geq 0$, then (2.6) is satisfied for $k = 3$. If $\delta \leq 0$, i.e. $\kappa \leq 2/(2\gamma + 1)$, then obviously $P(u, v, w) \geq \alpha > 0$. Next consider $\delta > 0$. Lemma 2.1 yields that $P(u, v, w) \geq 0$ whenever

$$(\delta + 1)(3 - 2\sqrt{\delta + 1}) \geq \frac{1}{2} \quad \text{and} \quad \delta \leq 1. \quad (2.7)$$

Set $x = \sqrt{\delta + 1}$. Then $x > 1$ and

$$(\delta + 1)(3 - 2\sqrt{\delta + 1}) \geq \frac{1}{2} \iff 4x^3 - 6x^2 + 1 \leq 0 \iff (2x - 1)(2x^2 - 2x - 1) \leq 0 \iff x \leq \frac{1}{2} + \frac{1}{2}\sqrt{3}.$$

It follows that (2.7) is equivalent to $\delta \leq \frac{1}{2}\sqrt{3}$, which means $\kappa \leq (2 + \sqrt{3})/(2\gamma + 1)$. Hence, if

$$\kappa \leq \min \left\{ 2, \frac{2 + \sqrt{3}}{2\gamma + 1} \right\},$$

then (2.6) holds for $k = 3$. Selecting the upper bound for κ , yields that (2.5b) is fulfilled for $k = 3$ whenever

$$\theta \geq \max \left\{ \frac{1}{4}, \frac{2\gamma + 1}{4 + 2\sqrt{3}} \right\}.$$

■

Upon setting $\gamma = 1$ in Theorem 2.3 the resulting sufficient conditions on θ for the CS, MCS, HV schemes agree with those in [11, Thms. 2.2, 2.5, 2.8]. The above theorem thus forms a proper generalization of results in [11]. For the Do scheme, the obtained sufficient condition generalizes and improves the corresponding result for this scheme from [3]. In particular, if $\gamma = 1$ and $k = 3$, then [3] yields $\theta \geq 3\sqrt{3} - \frac{9}{2} \approx 0.696$, whereas Theorem 2.3 yields $\theta \geq \frac{2}{3}$.

In view of Theorem 2.3, a smaller parameter value θ can be chosen while retaining unconditional stability if it is known that (1.2) holds with certain given $\gamma < 1$. This is useful, in particular since a smaller value θ often yields a smaller, i.e., more favorable, error constant.

The MCS scheme with the lower bound for θ given by Theorem 2.3 has been successfully used recently in the actual application to the three-dimensional Heston–Hull–White PDE from financial mathematics, see Haentjens & In 't Hout [6].

The following theorem provides, for each ADI scheme, a necessary condition on θ for unconditional stability.

Theorem 2.4 *Let $k \geq 2$ and $\gamma \in [0, 1]$ be given and consider any ADI scheme from Section 1. Suppose that the scheme is unconditionally stable whenever it is applied to a system (1.3), (1.4) that is obtained by central second-order FD discretization and splitting as described in Section 1 of any equation (1.1) with positive semidefinite $k \times k$ matrix D satisfying (1.2) and periodic boundary condition. Then θ must satisfy the following bound:*

- *Do scheme:*

$$\theta \geq \max \left\{ \frac{1}{2}, \frac{1}{2} d_k [(k-1)\gamma + 1] \right\} \quad \text{with} \quad d_k = \left(1 - \frac{1}{k} \right)^{k-1}$$

- *CS scheme:*

$$\theta \geq \max \left\{ \frac{1}{2}, \frac{1}{2} c_k k \gamma \right\} \quad \text{with} \quad c_k = \left(1 - \frac{1}{k} \right)^k$$

- *MCS scheme:*

$$\theta \geq \max \left\{ \frac{1}{4}, \frac{1}{2} b_k [(k-1)\gamma + 1] \right\} \quad \text{with} \quad b_k = \frac{1}{1 + \left(1 + \frac{1}{k-1} \right)^{k-1}}$$

- *HV scheme:*

$$\theta \geq \max \left\{ \frac{1}{4}, \frac{1}{2} a_k [(k-1)\gamma + 1] \right\}$$

$$\text{with } a_k \text{ the unique solution } a \in \left(0, \frac{1}{2} \right) \text{ of } 2a \left(1 + \frac{1-a}{k-1} \right)^{k-1} - 1 = 0.$$

Proof As in the foregoing proof, we consider here the HV scheme and leave the (analogous) proofs for the other three ADI schemes to the reader.

Consider the $k \times k$ matrix $D = (d_{ij})$ with $d_{ii} = 1$ and $d_{ij} = \gamma$ whenever $1 \leq i \neq j \leq k$. Clearly, D is symmetric positive semidefinite and (1.2) holds. Let $\Delta x_i \equiv \Delta x > 0$, so that $r_{ij} \equiv r := \Delta t / (\Delta x)^2$.

First, choose the angles ϕ_j in (1.17) equal to zero for $j \geq 2$. Then the eigenvalues z_j are given by $z_0 = 0$, $z_1 = -2r(1 - \cos \phi_1)$ and $z_2 = z_3 = \dots = z_k = 0$. In view of (2.5b), we have

$$2p - 1 + \frac{1}{2}(z_0 + z) = 1 + (\frac{1}{2} - 2\theta)z_1 \geq 0$$

whenever $r > 0$, $\phi_1 \in [0, 2\pi)$. This immediately implies $\theta \geq \frac{1}{4}$.

Next, choose all angles ϕ_j in (1.17) the same, i.e., $\phi_j \equiv \phi$. Then the eigenvalues z_j are given by

$$\begin{aligned} z_0 &= -rk(k-1)\gamma[\sin^2 \phi - \bar{\beta}(1 - \cos \phi)^2], \\ z_j &= -2r(1 - \cos \phi), \quad j = 1, 2, \dots, k, \end{aligned}$$

where

$$\bar{\beta} = \frac{\sum_{i \neq j} \beta_{ij}}{k(k-1)}.$$

Note that $|\bar{\beta}| \leq 1$. By (2.5b), it must hold that

$$\theta \geq -\frac{1}{2} \frac{\theta z_0 + \theta z}{2p - 1} = \frac{k}{2} \frac{(k-1)\gamma\theta r[\sin^2 \phi - \bar{\beta}(1 - \cos \phi)^2] + 2\theta r(1 - \cos \phi)}{2[1 + 2\theta r(1 - \cos \phi)]^k - 1}$$

whenever $r > 0$, $\phi \in [0, 2\pi)$. Setting $\alpha = 2\theta r(1 - \cos \phi)$, this yields

$$\theta \geq \frac{k}{2} \frac{(k-1)\gamma\alpha[1 + \cos \phi - \bar{\beta}(1 - \cos \phi)]/2 + \alpha}{2(1 + \alpha)^k - 1}$$

for all $\alpha > 0$, $\phi \in (0, 2\pi)$. Taking the supremum over ϕ , gives

$$\theta \geq \frac{1}{2} h(\alpha) [(k-1)\gamma + 1] \quad \text{for all } \alpha > 0,$$

where

$$h(\alpha) = \frac{k\alpha}{2(1 + \alpha)^k - 1}.$$

By elementary arguments (cf. [11]) it follows that the function h has an absolute maximum which is equal to a_k given in the theorem. ■

Upon setting $\gamma = 1$ in Theorem 2.4, the necessary conditions on θ for the CS, MCS, HV schemes reduce to those given in [11, Thms. 2.3, 2.6, 2.9]. Further, for the Do scheme and $\gamma = 1$ there is agreement with the necessary condition from [3].

It is readily verified that, for each ADI scheme, the sufficient conditions of Theorem 2.3 and the necessary conditions of Theorem 2.4 are identical whenever $k = 2$ or $k = 3$ and $0 \leq \gamma \leq 1$. Hence, in two and three spatial dimensions, these conditions are sharp.

The interesting question arises whether the necessary conditions of Theorem 2.4 are also sufficient in spatial dimensions $k \geq 4$. In [11] it was proved that this is true for the HV scheme and $\gamma = 1$. It can be seen, however, that the proof from [11] does not admit a straightforward extension to values $\gamma < 1$. Further, in the case of the Do, CS, MCS schemes a proof is not clear at present. Accordingly, we leave this question for future research.

3 Numerical illustration

In this section we illustrate the main results of this paper, Theorems 2.3 and 2.4. We present experiments where all four ADI schemes (1.5)–(1.8) are applied in the numerical solution of multidimensional diffusion equations (1.1) possessing mixed derivative terms. The PDE is semidiscretized by central second-order finite differences as described in Subsection 1.3, with $\beta_{ij} \equiv 0$, and the semidiscrete matrix A is splitted as described in Subsection 1.2. The boundary condition is taken to be periodic (in this case $g(t) \equiv 0$).

The first experiment deals with (1.1) in two spatial dimensions. We choose initial function

$$u(x_1, x_2, 0) = e^{-4[\sin^2(\pi x_1) + \cos^2(\pi x_2)]} \quad (0 \leq x_1, x_2 \leq 1)$$

and diffusion matrix D given by

$$D = 0.025 \begin{pmatrix} 1 & 2\gamma \\ 2\gamma & 4 \end{pmatrix}.$$

This matrix D is positive semidefinite and the condition (1.2) holds whenever $\gamma \in [0, 1]$. Consider $\gamma = 0.9$. Then the lower bounds on θ provided by Theorem 2.3 for the MCS and HV schemes are, rounded to three decimal places, equal to 0.317 and 0.278, respectively. For the Do and CS schemes, the lower bound always equals $\frac{1}{2}$ in two spatial dimensions, independently of γ .

Figure 1 shows for $\Delta x_1 = \Delta x_2 = 1/80$ the semidiscrete solution values $U(0)$ and $U(5)$ displayed on the grid in Ω , so that they represent the exact solution u at $t = 0$ and $t = 5$.

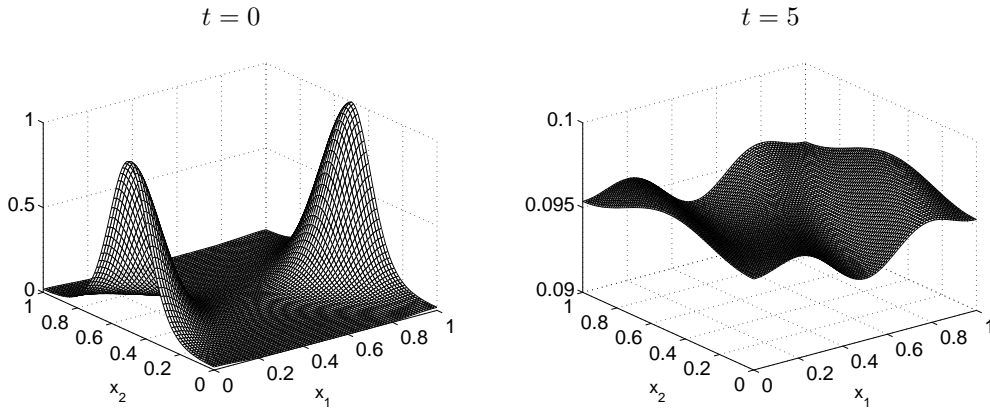


Figure 1: Exact solution u of 2D problem at $t = 0$ and $t = 5$. Note the different scales on the vertical axes.

To the semidiscrete systems with $\Delta x_1 = \Delta x_2 = 1/m$ for $m = 40, 80$ we have applied the Do, CS, MCS, HV schemes using their exact lower bound values θ (above) as well as the values 0.45, 0.45, 0.29, 0.25, respectively, which are approximately 90% of these. For a sequence of step sizes $\Delta t = 1/N$ with $10^{-3} \leq \Delta t \leq 10^0$ we computed the *global temporal errors* at time $t = 5$, defined by

$$e(\Delta t; m) = m^{-1} \|U(5) - U_{5N}\|_2,$$

where $\|\cdot\|_2$ is the Euclidean vector norm and $1/m$ is a normalization factor. Figure 2 displays the obtained result.

From the right column of Figure 2 it is clear that, for each ADI scheme, using the smaller value θ leads to large temporal errors for natural step sizes. We verified that these large errors correspond to the spectral radii of the pertinent iteration matrices being greater than 1. This indicates that they are caused by a lack of stability. Additional experiments with larger values t (e.g. $t = 10$) also shows that the large temporal errors are amplified, as one may expect.

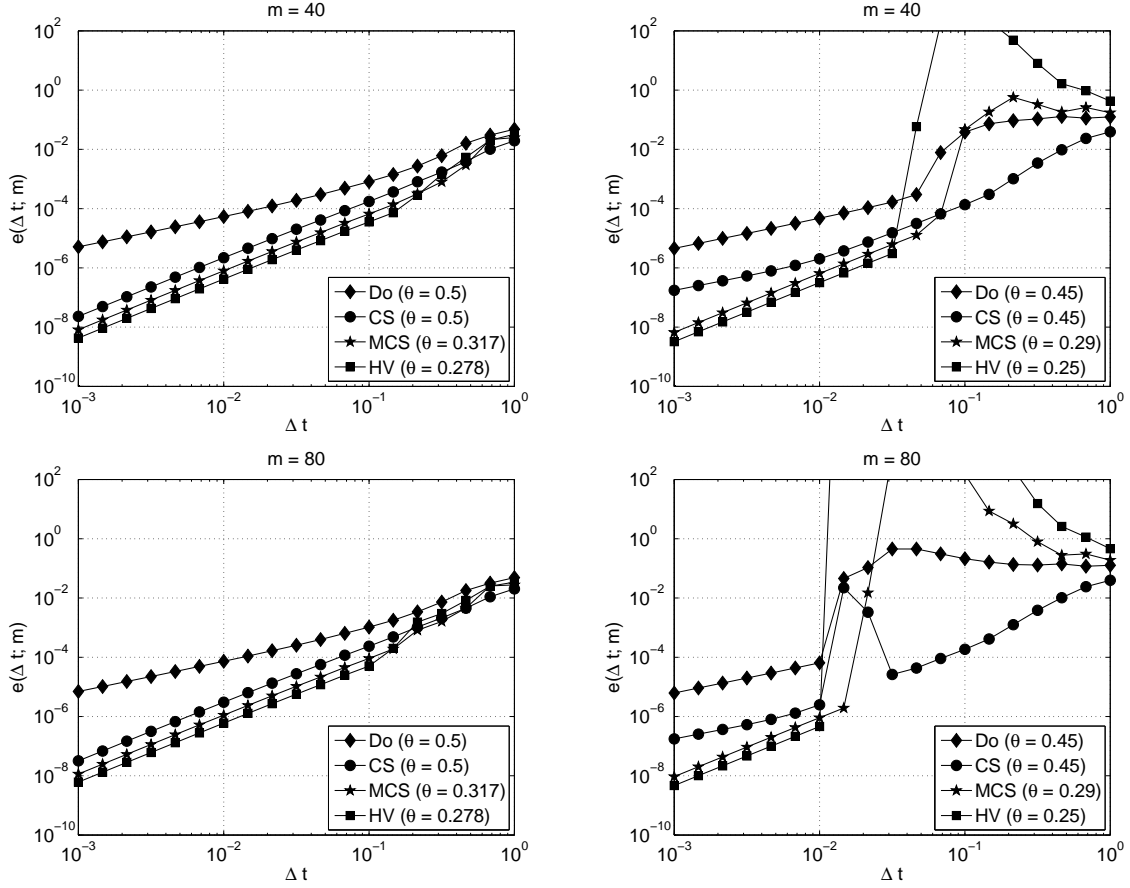


Figure 2: Global temporal errors $e(\Delta t; m)$ versus Δt for Do, CS, MCS, HV schemes when applied to a semidiscretized 2D problem (1.1) with $\gamma = 0.9$. Top row: $m = 40$. Bottom row: $m = 80$. Left column: lower bound values θ given by Theorem 2.3. Right column: values θ that are about 90% of these.

The left column of Figure 2 displays the results in the case where the lower bound values θ , given by Theorem 2.3, are used. Then all temporal errors are bounded from above by a moderate constant and decrease monotonically when Δt decreases. This suggests an unconditionally stable behavior of the schemes. A further examination in this case shows that the global temporal errors for the Do scheme can be bounded from above by $C\Delta t$ and for the CS, MCS, HV schemes by $C(\Delta t)^2$ (whenever $\Delta t > 0$) with constants C depending on the scheme. This clearly agrees with the respective orders of consistency of the schemes. Moreover, for each scheme the constant C is only weakly dependent on the number of spatial grid points, determined by m , indicating that the error bounds are valid in a stiff, hence favorable, sense. We remark that similar conclusions were found for larger values t . Further we numerically verified that upon increasing θ from its lower bound value, the error constant C increases, as mentioned in the discussion following Theorem 2.3.

The second experiment deals with (1.1) in three spatial dimensions. We take initial function

$$u(x_1, x_2, x_3, 0) = e^{-[\cos^2(\pi x_1) + \cos^2(\pi x_2) + \cos^2(\pi x_3)]} \quad (0 \leq x_1, x_2, x_3 \leq 1)$$

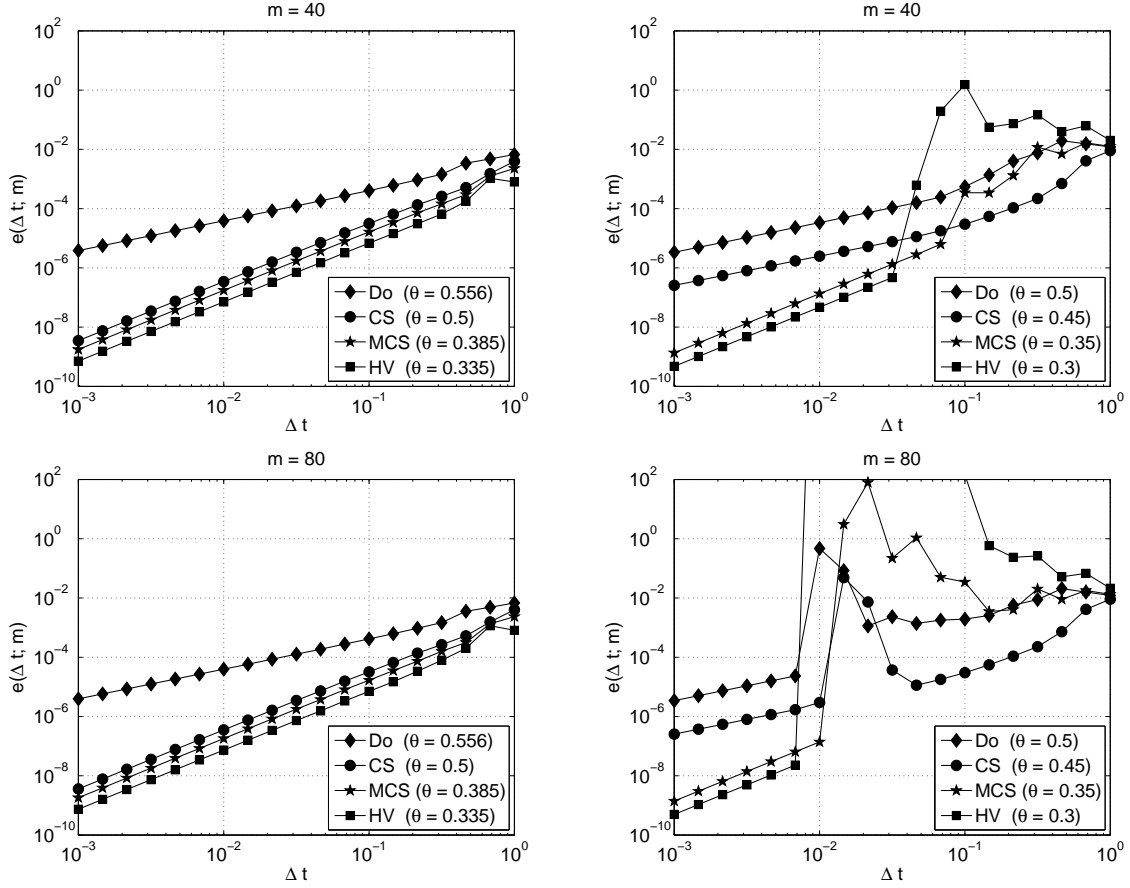


Figure 3: Global temporal errors $e(\Delta t; m)$ versus Δt for Do, CS, MCS, HV schemes when applied to a semidiscretized 3D problem (1.1) with $\gamma = 0.75$. Top row: $m = 40$. Bottom row: $m = 80$. Left column: lower bound values θ given by Theorem 2.3. Right column: values θ that are about 90% of these.

and diffusion matrix D given by

$$D = 0.025 \begin{pmatrix} 1 & 2\gamma & \gamma \\ 2\gamma & 4 & 2\gamma \\ \gamma & 2\gamma & 1 \end{pmatrix},$$

which is positive semidefinite and such that condition (1.2) holds whenever $\gamma \in [0, 1]$. Here we take $\gamma = 0.75$. Then the lower bounds on θ given by Theorem 2.3 for the Do, MCS, HV schemes are, rounded to three decimal places, equal to 0.556, 0.385, 0.335, respectively. For the CS scheme the lower bound is always $\frac{1}{2}$ in three spatial dimensions, independently of γ . To the semidiscrete systems with $\Delta x_1 = \Delta x_2 = \Delta x_3 = 1/m$ for $m = 40, 80$ we have applied the Do, CS, MCS, HV schemes using their exact lower bound values θ as well as the values 0.5, 0.45, 0.35, 0.3, respectively, which are approximately 90% of these. Figure 3 displays the normalized global temporal errors

$$e(\Delta t; m) = m^{-3/2} |U(5) - U_{5N}|_2$$

for a sequence of step sizes $\Delta t = 1/N$ with $10^{-3} \leq \Delta t \leq 10^0$. Exactly the same observations can be made as in the experiment (above) for the two-dimensional case. The large temporal errors for each ADI scheme when applied with the smaller value θ , as seen in the right column of Figure 3, correspond to instability of the scheme. When applied with their lower bound values θ , given by

Theorem 2.3, the error behavior for all ADI schemes is in agreement with unconditional stability of the schemes. Moreover, in this case a stiff order of convergence is observed that is equal to one for the Do scheme and equal to two for the CS, MCS and HV schemes.

4 Conclusions

In this paper we analyzed stability in the von Neumann sense of four well-known ADI schemes - the Do, CS, MCS and HV schemes - in the application to multidimensional diffusion equations with mixed derivative terms. Such equations are important, notably, to the field of financial mathematics. Necessary and sufficient conditions have been derived on the parameter θ for unconditional stability of each ADI scheme by taking into account the actual size of the mixed derivative terms, measured by the quantity $\gamma \in [0, 1]$. Our two main theorems generalize stability results obtained by Craig & Sneyd [3] and In 't Hout & Welfert [11]. Ample numerical experiments have been presented, illustrating the main theorems and also providing insight into the convergence behavior of all schemes.

Among issues for future research, it is of much interest to derive sufficient conditions on θ for unconditional stability of each ADI scheme in arbitrary spatial dimensions $k \geq 4$ and arbitrary $\gamma \in [0, 1]$. Also, it is of much interest to extend the results obtained in this paper to equations with advection terms. This leads to general complex, instead of real, eigenvalues, which forms a nontrivial feature for the analysis, cf. e.g. [9, 10].

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